

# NEW METHODOLOGY FOR OPTIMIZATION OF FRESHWATER INFLOWS TO ESTUARIES

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**ABSTRACT:** The objective of this work is to develop a general methodology for determination of the optimal freshwater inflows into bays and estuaries to balance freshwater demands with the harvest of various types of estuarine resources. The methodology is based upon solving a large-scale nonlinear programming problem formulated in an optimal-control framework. Constraints of the optimization problem include regression equations for harvest of the various species that express fishery harvest as a function of the quantity of freshwater inflow. The stochastic element of the problem (i.e. the uncertainty associated with the regression equations for harvest) is considered by expressing constraints in a chance-constrained formulation. A nonlinear programming optimizer is interfaced with a hydrodynamic transport model to implicitly solve the hydrodynamic-salinity constraint equations for salinity levels. An augmented Lagrangian method is introduced to incorporate the salinity constraints into the objective so that the problem size for the optimizer is significantly reduced. A computer model OPTFLOW has been developed by interfacing a simulator for the hydrodynamic-salinity (HYD-SAL) with a nonlinear optimizer (GRG2) to apply the methodology by the present writers in an accompanying companion paper. An efficient approximation scheme is developed for evaluation of the objective function and its reduced gradient to reduce the computational effort dramatically. The new methodology can provide a very useful tool for decision makers to quantitatively analyze various water-management strategies.

## PROBLEM IDENTIFICATION

Freshwater is one of the most precious natural resources in many areas of the United States, especially the Gulf Coast states and California, and elsewhere in the world. Freshwater inflow needed to maintain the healthy ecological conditions of coastal estuaries must compete with the demands upstream such as municipal, industrial, and agricultural users. Estuaries provide areas of nursery habitats for juvenile forms of marine species, for sport and commercial fishing, and for other recreational activities. The provision of sufficient freshwater inflows to estuaries is a vital factor in maintaining estuarine productivity. The desired approach to water-resources management is to optimize flow into the estuary (by minimizing the total volume of flow, or by maximizing the diversions and storage within limits of water rights and capacity, or both), while preserving an acceptable habitat in specific regions of the estuary to accommodate the requirements of key organisms. Salinity is an index that has been well established to indicate ecological conditions in an estuary because it measures the relative proportion of freshwater to seawater. Salinity not only reflects the ratio of freshwater to seawater but also provides other information such as nutrient supply, sediment, and components of the food web.

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A key element in developing an optimization problem is the mathematical relation between salinity in the estuary and flow,  $s = F(Q)$ . Usually the relation is based upon statistical association, i.e. a regression form established from field data. The Texas Water Development Board (TWDB) ("Hydrological" 1978; "Mathematical" 1979; "Lavaca" 1980) has made particularly extensive application of this approach in establishing freshwater inflow requirements, as a part of its bays and estuaries program. The statistical regression  $s = F(Q)$  proves to be extremely noisy because of the variability in salinity. In the case of the Texas bays, nearly the entire possible range of salinity values can be found in the historical field data for any given value of concurrent inflow. The reasons for this are threefold. First, the value of salinity in a given region of the bay is dependent on several other factors in addition to freshwater inflow, notably the various hydrodynamic circulation processes including tides, responses of the bay to meteorological forcing, and the effect of density currents particularly operating in conjunction with deep-draft ship channels. Second, the time scale of response of salinity is typically much longer than the variability of freshwater inflow. The value of salinity is the integrated response to perhaps several months of the freshwater inflow "signal." Salinity is also a function of spatial location within an estuary. Generally, salinity is low near the river inlet (upper estuary) and high near the ocean outlet (lagoonal arm of the estuary). The regressional function  $s = F(Q)$ , at best, only reflects the averaged salinity conditions.

It should also be noted that the optimization problem is in fact time varying, primarily because the salinity requirements of key organisms in the estuary will vary with season through the year, depending upon the life stage of the organism and its presence or absence within the estuary. (Many of the important commercial species are anadromous, migrating into or out of the estuary.) The salinity limits for a specific organism are based on the statistical association between the presence of that organism in the estuary (as reflected in catch data or harvest data) and salinity, or on the physiological dependence on salinity as revealed in laboratory studies. Thus far, the optimization problem has only been treated on a steady-state basis (Martin 1987; Bao et al. 1989; Tung et al. 1990). Accommodation of the seasonal variation in salinity requirement was made by the TWDB by subdividing the year into several seasons and solving the steady-state problem separately for each season.

The essential weakness in the preceding formulation is that the salinity regression equations are too simple to represent the complicated hydrodynamic transport physical process coupling salinity, inflows, and other factors. The present paper reformulates the problem, replacing the statistical regression  $s = F(Q)$  with a mathematical model of hydrodynamic transport, relating salinity at a given point in the estuary to a time-varying boundary condition of riverine inflow. Such an approach has the following advantages:

1. More accurate and self-consistent definition of salinity as a function of flow, enabling greater precision in the optimization results.
2. Explicit incorporation of physical processes other than freshwater inflow affecting salinity in the real system, including tides, meteorology, and internal circulations.
3. The ability to accommodate time variation in the response of salinity to freshwater inflow, so as to readily generalize to the full time-varying

problem (although the optimization problem can also be solved in a steady-state framework with steady inflows).

4. The ability to accommodate generalization to full time variation in upstream water demands, including seasonality of irrigation and long-term demographic changes.

5. The ability to consider either averaged inflow, prespecified scenarios of inflow, or long-term simulations using real hydrological data.

In some estuaries, a direct measure of organism abundance is available in the data on commercial fishery landings taken from the estuary. This “harvest” data can be employed as an index of populations of key organisms and analyzed statistically to establish its dependence on freshwater inflow,  $H_k = f(Q)$ . While this might appear superior to the indirect salinity-index approach, the causal connection between flow and harvest may be obscured by unmeasurable parameters of the fishing process such as effort, selectivity, and skill, and may be corrupted by poor reporting or the difference between locality of landing (i.e. port) and locality of catch, to say nothing of other environmental variables unrelated to inflow. This regression therefore tends to be noisy and statistically uncertain. On the other hand, it is directly pertinent to the problem, and when the data are available, should be accommodated within the optimization problem, either as an objective function or as a constraint. To account for the uncertainty of the regression these equations can be rewritten as chance constraints (see Appendix I). Thus, the stochastic constraints are transformed into probabilistic statements to indicate the probability that the constraint will be satisfied within a specified reliability level.

**Overview**

The overall optimization model can be stated in the following general nonlinear programming format using an objective function to minimize freshwater inflows or to maximize fishery harvest:

$$\text{Optimize } f(\mathbf{Q}, \mathbf{s}, \mathbf{H}) \dots\dots\dots (1)$$

subject to the following constraints:

First, hydrodynamic transport equations that relate salinity  $\mathbf{s}$  (vector in spatial and temporal domains) to the freshwater inflow  $\mathbf{Q}$

$$\mathbf{G}(\mathbf{Q}, \mathbf{s}) = 0 \dots\dots\dots (2)$$

where  $\mathbf{Q}$  = a vector of the independent variable (control variable) as a function of time; and  $\mathbf{s}$  = a vector of the dependent variable (state variable) as a function of time and location.

Second, regression equations that relate inflow to fish harvest

$$\mathbf{h}(\mathbf{Q}, \mathbf{H}) = 0 \dots\dots\dots (3)$$

where  $\mathbf{H}$  = a vector of the fish harvest for different species.

Third, constraints that define limitations on freshwater inflows due to upstream demands and water uses, and historical ranges

$$\mathbf{Q} \leq \mathbf{Q} \leq \bar{\mathbf{Q}} \dots\dots\dots (4)$$

where  $\mathbf{Q}$  and the limitations are defined in the general terms so that they can be interpreted as monthly, seasonal, and annual flows. The marsh in-

undation requirements are also included in this expression, which are basically lower bounds on flows during certain time periods.

And fourth, constraints that define limitations on salinity

$S \leq S \leq \tilde{S}$  ..... (5)

The problem posed is a discrete time optimal control problem in which the constraints that relate the state variables (salinities) to the control variables (freshwater inflows) are solved implicitly by the simulator, hydrodynamic-salinity (HYD-SAL). For each iteration in the process of the optimization, the optimizer computes the new values of control variables and passes that information to the simulator to update the corresponding state variables. A reduced optimization problem is then formed with a smaller number of decision variables and constraints. The control variables are the freshwater inflows as a function of time. The state variables are the salinities as a function of time and location in the bay and estuary. During each iteration of the optimizer, a set of control or decision variables, the freshwater inflows for each time period, are sent to the simulator, as shown in Fig. 1. The purpose of the estuarine hydrodynamic transport model is to simulate the flow circulation in the bay system and to be able to compute the spatial distribution of salinity in the bay for the time period of interest for given freshwater inflows and other boundary conditions. The hydrodynamic transport model then solves for the salinities for each location in the bay and estuary at each time period. Basically, the state variables (salinities) and the control variables (freshwater inflows) are related through the hydrodynamic transport model. In essence, the simulator equations are used to express the states in terms of the controls yielding a much smaller nonlinear optimization problem.

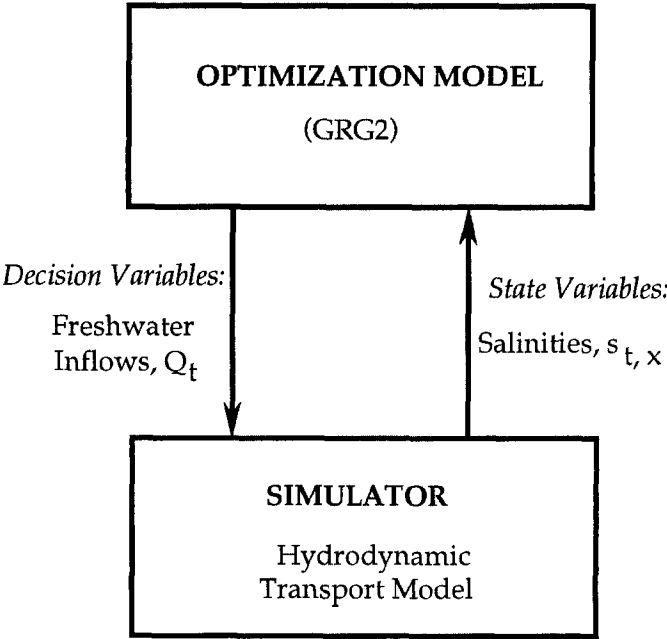


FIG. 1. Optimizer-Simulator Interface

## Hydrodynamic Transport Simulator for Estuaries

The essence of the present paper is to develop a general methodology for the estuarine freshwater resources management so that for discussion purposes the hydrodynamic transport model needed for simulation of temporal and spatial variation of salinity is not restricted to a particular model. The selection of an appropriate model depends on a number of factors such as efficiency, accuracy, complexity, and availability of the model. Even if a desired hydrodynamic transport model has been chosen and applied in the simulation, a better model can always be used to replace it in the future as more efficient models are developed. The formulation of hydrodynamic and transport-governing equations varies slightly for each model depending on the various assumptions and approximations introduced. The model used for discussion purposes in the application in this research is a two-dimensional, finite-difference model referred to as HYD-SAL ("Lavaca" 1980). Such a model is used as an example for the formulation of governing equations and their finite-differencing approximations (Fig. 2).

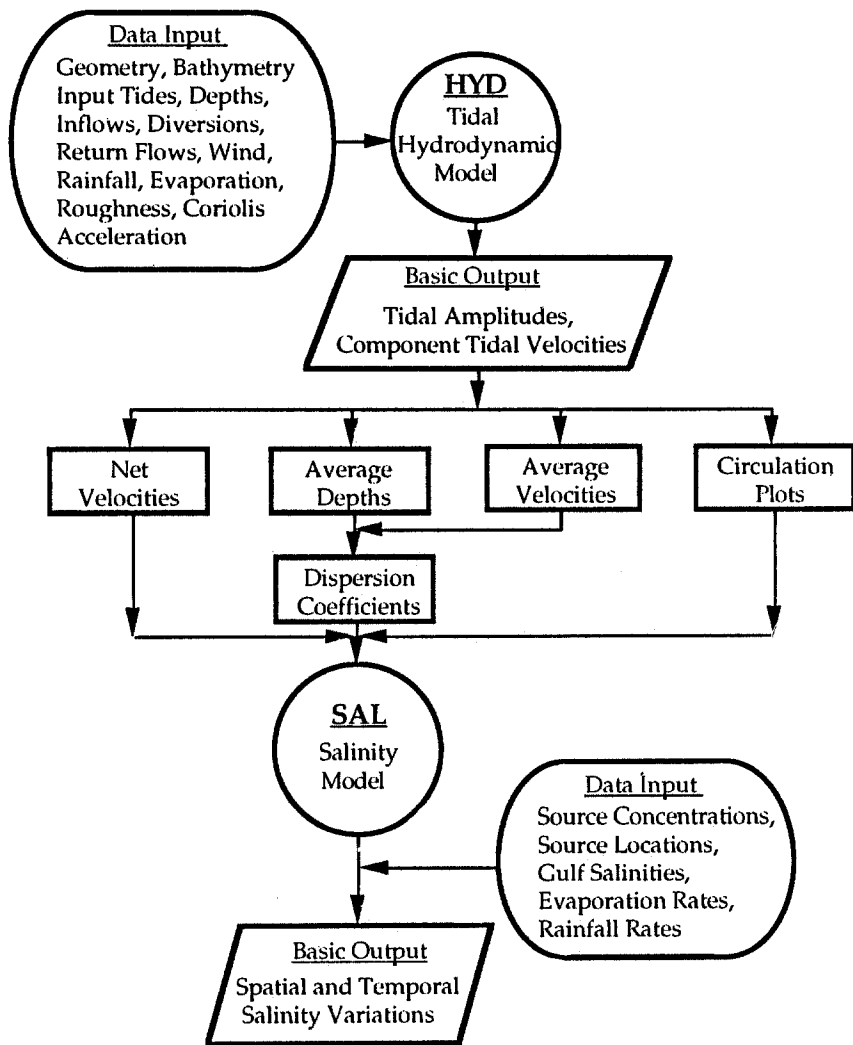
One of the key elements of the methodology is the determination of salinity levels in the estuary defined in terms of a particular sequence of inflows. The hydrodynamic model embedded within this procedure should satisfy the following desired criteria.

- The model should be capable of representing an estuarine system with complex circulation, to offer a fair level of complexity in the salinity-inflow relation and therefore in the optimization methodology
- The model should be capable of exhibiting a significantly filtered response to time variations in freshwater inflow, including time lags and inertia, to differentiate the salinity-inflow association from the simple regression forms used in past studies
- The model should be representative of a real estuarine system, so as to allow demonstration of the methodology in a case-study format
- The model should facilitate generalization to a more sophisticated high-resolution estuarine model for detailed applications of the optimization methodology

In addition to the general requirements for an estuarine hydrodynamic model, the following criteria are considered, in the following order of priority, when selecting a simulation model:

1. The hydrodynamic transport model needs to be called by the optimizer so frequently that the most restrictive requirement for a suitable simulation model is the speed of execution of the code.
2. The model should be capable of representing an estuarine system with complex circulation, temporal, and spatial salinity variability.
3. The model should be capable of simulating long-term salinity values such as monthly averaged salinity in the bay system.

The preceding requirements can be met for most applications using a two-dimensional horizontal depth-averaged tidal hydrodynamic transport model, implemented for one of the Texas bays. The computational model to be employed is one of several models currently available. These include the finite-difference models developed in the Galveston Bay project (Ward



**FIG. 2. Relationship between Tidal Hydrodynamic and Salinity Models**

and Espey 1971), the finite-difference models developed by the Texas Water Development Board for the Texas bays ("Lavaca" 1980), the finite-difference model developed by the Rand Corp. (Leendertse 1967a, b; Ward and Espey 1971), and the quasi-two-dimensional finite-difference dynamic estuary model (DEM) developed for the Sabine Lake estuarine system (Brandes et al. 1975). The available two-dimensional (2D) finite-element models tested for selection are FESWMS-2DH (Froehlich 1989), GEVIS (Lynch and Gray 1979), and TXBLEND (Matsumoto 1992).

The governing equations for the 2D horizontal model are the vertical-

averaged equations of momentum, continuity, and salinity mass budget: the momentum equation in  $x$ -direction

$$\frac{\partial q_x}{\partial t} - \Omega q_y = -gd \frac{\partial h}{\partial y} - fqq_x + X_w \dots\dots\dots (6)$$

the momentum equation in  $y$ -direction

$$\frac{\partial q_y}{\partial t} - \Omega q_x = -gd \frac{\partial h}{\partial y} - fqq_y + Y_w \dots\dots\dots (7)$$

the continuity equation

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial h}{\partial t} = r - e \dots\dots\dots (8)$$

and the conservation (transport) equation

$$\frac{\partial s}{\partial t} + \frac{\partial (Us)}{\partial x} + \frac{\partial (Vs)}{\partial y} = \frac{\partial}{\partial x} E_x \frac{\partial s}{\partial x} + \frac{\partial}{\partial y} E_y \frac{\partial s}{\partial y} \dots\dots\dots (9)$$

where  $t$  = time;  $x$  and  $y$  = horizontal Cartesian coordinates;  $q_x$  and  $q_y$  = depth-averaged flow components in the  $x$ - and  $y$ -directions per unit width;  $\Omega$  = Coriolis parameter equal to  $2\omega \sin \phi$ ;  $\omega$  = angular rotation of the earth;  $\phi$  = latitude;  $g$  = gravitational acceleration;  $h$  = water surface elevation;  $d$  = water depth equal to  $h - z$ ;  $z$  = bottom elevation;  $f$  = bottom friction term from the Manning equation;  $q$  = flow per unit width equal to  $\sqrt{q_x^2 + q_y^2}$ ;  $X_w$  = wind stress per unit density of water in the  $x$ -direction equal to  $KV_w^2 \cos \theta$ ;  $Y_w$  = wind stress per unit density of water in  $y$ -direction equal to  $KV_w^2 \sin \theta$ ;  $K$  = a wind stress coefficient;  $V_w$  = wind velocity at 10 m above the water surface;  $\theta$  = wind direction with respect to the  $x$ -axis;  $r$  = rainfall intensity;  $e$  = evaporation rate;  $U$  and  $V$  = net velocities over a tidal cycle;  $s$  = vertically-averaged salinity; and  $E_x$ ,  $E_y$  = horizontal dispersion coefficients in the  $x$ - and  $y$ -directions, respectively.

In the momentum equations, the advective terms are neglected and the water density is treated as a constant. The assumption of constant density considerably simplifies the governing equations by decoupling salinity from the momentum equations, but at the expense of neglecting salinity-induced accelerations. The remaining terms in the momentum equations are the inertia, the Coriolis acceleration, gravity, friction, and wind stress. The precipitation and evaporation terms are also added in the continuity equation for the mass conservation. The transport equation is a linear second-order partial differential equation for convective-dispersion.

Boundary conditions are imposed around the periphery of the estuary including water-land boundaries, partial internal boundaries (e.g. submerged reefs for hydrodynamic equations only), freshwater flows (e.g. river flows, diversions, and return flows), and open saltwater ocean boundaries (tidal excitation). For salinity,  $s = s_0$  imposed at the ocean boundaries, a von Neumann condition (zero flux) at land boundaries, and an open-boundary condition at the inflow points. These boundary conditions can be a function of time.

The hydrodynamic equations are nonlinear first-order partial differential equations to solve for three unknowns: flow fluxes in the  $x$ - and  $y$ -directions and water-surface elevation ( $q_x$ ,  $q_y$ , and  $h$ ). A fully explicit method is used for solving the hydrodynamic equations in HYD-SAL that is a time-centered

difference scheme involving time stepping of the “leap frog” type for computations of flows and water surface elevations. Fig. 2 shows the relationship between the tidal hydrodynamic model and salinity model.

The initial hydrodynamics can be either set as zero (default in model) or read from input data if they are known. Since the simulator is carried out for an entire year, simulation is only the first month the hydrodynamics are set as default values and the antecedant conditions are used for the simulation of the rest of the months of the year. Similarly, the initial salinity conditions can be either set as a uniform known distribution. However, depending on the availability of hydrodynamic and salinity data and the purpose of application, the salinity transport model can be steady-state or unsteady-state. For instance, in the application of this model (Bao and Mays 1994), a two-cycle tidal data, which is averaged from one of month data to represent the tidal condition for that month, is used in the hydrodynamic simulations. Accordingly, the default salinity (uniform value) is used for the first month and the transport model (SAL) is run until steady-state conditions are reached. The final salinity values are the solutions of the salinities in that month and used as initial salinities for simulation of the next month.

### Reduced Problem

For illustration purposes, the objective to minimize the total annual freshwater inflow, is selected to demonstrate the formulation of the optimization problem and solution procedure. The independent (decision) variables are the monthly averaged freshwater inflows from each river connected to the bay system. Thus, even in the original general format the objective function (5) is a function of the flow vector  $\mathbf{Q}$  only. The problem formulated next, however, is still defined as the “reduced” problem for the reasons that: First, it can be viewed as the coefficients associated with a (salinity vector) terms in the objective function are set to zero; second, the size of the optimization problem is dramatically reduced because the  $\mathbf{G}$  constraints in (2) are solved implicitly by the hydrodynamic transport simulator; and third, this notation makes it more convenient for the description of model formulation and structure hereafter. The reduced problem consists of the “reduced” objective function

$$\text{minimize } f[\mathbf{Q}, s(\mathbf{Q})] = \min F(\mathbf{Q}) \dots\dots\dots (10)$$

subject to harvest constraints (3), bounds (4), and salinity bounds (5).

### Solution Procedure

To force satisfaction of the salinity bound constraints in the optimizer, these bounds on the state variables (salinities) are incorporated into the objective function using the augmented Lagrangian algorithm. Such an approach not only forces the state bounds to be satisfied, but also reduces the number of constraints. Since only inequality bound-type salinity constraints need to be incorporated, the objective function with the augmented Lagrangian function is expressed as

$$\min L[s(\mathbf{Q}), \mathbf{Q}, \mu, \sigma] = F(\mathbf{Q}) + \frac{1}{2} \sum \sigma_i \left[ \min \left( 0, c_i = \frac{\mu_i}{\sigma_i} \right) \right]^2 - \frac{1}{2} \sum_i \frac{\mu_i^2}{\sigma_i} \dots\dots\dots (11)$$

where  $i$  = index for each bound constraint;  $\sigma_i$  and  $\mu_i$  = penalty weights

and Lagrangian multipliers, respectively, for the  $i$ th bound; and  $c_i$  = violation of the bounds either above or below the minimum defined as

$$c_i = \min(s_i - \underline{s}_i, \bar{s}_i - s_i) \dots\dots\dots (12)$$

The reduced optimization problem with augmented Lagrangian terms for minimizing freshwater inflows is stated with the objective (11) is as follows:

$$\text{minimize } L[s(Q), Q, \sigma, \mu] \dots\dots\dots (13)$$

subject to

$$h[Q, s(Q), H] = 0 \dots\dots\dots (14)$$

and

$$Q \leq Q \leq \bar{Q} \dots\dots\dots (15)$$

which are, respectively, the constraints on harvest and the bounds on the freshwater inflows. The solution to this reduced problem is a two-step procedure. The overall problem is

$$\min_{\sigma, \mu} \left\{ \min_{Q \in Q_s} L[s(Q), Q, \mu, \sigma] \right\} \dots\dots\dots (16)$$

where  $Q_s$  = range of feasible freshwater inflows as given by (15). For given values of vectors  $\sigma$  and  $\mu$ , the reduced problem, (13), (14) and (15), are then solved using a nonlinear optimizer, such as GRG2 (Lasdon and Waren 1989), which is based upon the generalized reduced gradient method. The outer problem is iterated by updating the values of  $a$  and for the next solution run of the inner problem. The overall optimization is attained when  $\sigma$  and  $\mu$  both converge.

The updating formula used for  $\mu$  is:

$$\mu_i^{(k+1)} = \mu_i^{(k)} - \sigma_i c_i \text{ if } c_i < \frac{\mu_i}{\sigma_i} \dots\dots\dots (17a)$$

$$\mu_i^{(k+1)} = 0 \text{ otherwise} \dots\dots\dots (17b)$$

where  $k$  = number of the current iteration. The value of  $\sigma_i$  is adjusted once during early iterations and then kept constant.

The overall solution procedure is further illustrated through the flowchart in Fig. 3. There are two loops in this procedure, with the outer loop determining the Lagrangian multipliers (dual variables) and penalty weights. The inner loop solves the reduced augmented Lagrangian problem using the optimizer, GRG2, whose dual variables and penalty weights are fixed at the values determined by the outer loop. Once an inner loop is finished, the convergence criterion is checked by looking at the size of the salinity-bound infeasibility. If it is small enough, the procedure terminates; otherwise, the procedure returns to the outer loop and updates the dual variables and penalty weights and then goes to the inner loop and solves the new reduced augmented Lagrangian again with the updated  $\mu$  and  $\sigma$  from the outer loop. This process continues until a solution of the overall problem is found. Obviously there is no guarantee of convergence to a global optimum solution; however, with the use of initial trial solutions and engineering judgement optimal solutions can be found.

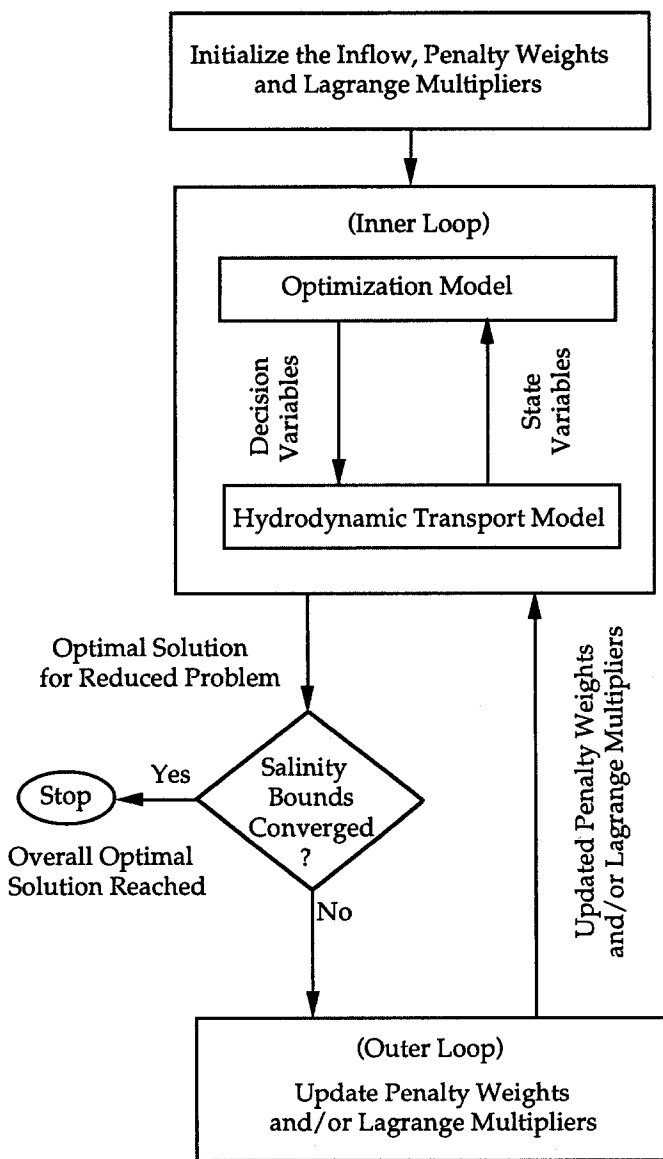


FIG. 3. Overall Solution Procedure

### Computation of Reduced Gradients of AL Problem

The augmented Lagrangian (AL) function, (11), is a function of flow  $\mathbf{Q}$ , salinity  $s(\mathbf{Q})$ , and Lagrangian parameters  $\sigma$  and  $\mu$ , which is also expressed as follows:

$$\min L[s(\mathbf{Q}), \mathbf{Q}, \boldsymbol{\mu}, \boldsymbol{\sigma}] = f(\mathbf{Q}) + \sum_i 1_i \{c_i[s(\mathbf{Q})], \mu_i, \sigma_i\} \dots\dots\dots (18)$$

where

$$\sum_i 1_i(\mathbf{s}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \sum_i = -\mu_i c_i(s_i) + \frac{1}{2} \sigma_i [c_i(s_i)]^2, \quad \text{if } c_i(s_i) < \frac{\mu_i}{\sigma_i} \dots (19a)$$

$$\sum_i 1_i(\mathbf{s}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \sum_i = \frac{1}{2} \frac{\mu_i^2}{\sigma_i}, \quad \text{if } c_i(s_i) \geq \frac{\mu_i}{\sigma_i} \dots (19b)$$

and the salinity violation vector  $\mathbf{c}$ , is a function of salinity  $\mathbf{s}$ , and the salinity bounds (12). From (12), the salinity violation term  $c_i(s) = c_i(s_i)$  or  $c_i(s) = c_i[s_i(\mathbf{Q})]$ . The gradients of the augmented Lagrangian function can be derived by applying the chain rule:

$$\frac{\partial L}{\partial \mathbf{Q}} = \frac{\partial f}{\partial \mathbf{Q}} + \sum_i \frac{\partial 1}{\partial c_i} \frac{\partial c_i}{\partial s_i} \frac{\partial s_i}{\partial \mathbf{Q}} \dots (20)$$

where  $(\partial 1/\partial c_i) =$  a function of  $\sigma$  and  $\mu$ . Hence,  $(\partial 1/\partial c_i)$  is constant for the inner optimization problem. From (12),  $\partial c_i/\partial s_i$  is either 1 or  $-1$ . Thus, the key component for the computation of the (reduced) gradients of the augmented Lagrangian is the partial derivatives of the salinity with respect to the monthly flow,  $\partial s/\partial \mathbf{Q}$ .

The spatial and temporal salinities in the bay system are computed by solving the simulator. The freshwater inflows  $\mathbf{Q}$  are part of the boundary conditions (water-land boundaries) for the hydrodynamic model and the salinity values in the river inlets are part of the boundary conditions for the transport model (source concentration boundaries). To compute the matrix  $\partial s/\partial \mathbf{Q}$  analytically, a new set of simulator equations need to be derived and the analytical solution may be very difficult, if it is not impossible. In this research, the computation of  $\partial s/\partial \mathbf{Q}$  is carried out by finite-difference methods either the forward differencing or the central differencing. More specifically,  $\partial s/\partial \mathbf{Q}$  is computed by perturbation of  $\mathbf{Q}$  and running the hydrodynamic transport simulator repeatedly.

The computation of the reduced gradient is done by the forward difference or the central difference method through calling of the hydrodynamic transport model to simulate the temporal and spatial salinity variability in the nonlinear optimizer. To update the objective function, 12 calls to the hydrodynamic transport simulator are required with each simulating for a period of one month.

Theoretically, for an estuary with two major river systems if the central difference is used, it requires  $24 \times 12 \times 2 = 576$  calls of the hydrodynamic transport simulator to update the AL reduced gradients, where 24 is the number of decision variables (monthly river flows); 12 is the number of months to be simulated for each variable ( $\mathbf{Q}$ ) to be perturbed to obtain  $\partial L/\partial \mathbf{Q}$ , which is on an annual basis, (20), and 2 results from the fact that the central difference requires monthly flows to be perturbed at both sides for computation of the AL reduced gradients. Although the number estimated for the simulation requirement can be reduced by 50% by running the simulation only for the remaining months, 288 calls of the simulator are still extremely expensive for only updating the AL gradients once.

The simulation results using HYD-SAL indicate that the impact of a monthly flow perturbation in months on the salinities in the bay system for the remaining months ( $t = t + 1, t + 2, \dots 12$ ) is so small that might be mainly affected due to the numerical computation errors (less than  $10^{-8}$ ). Therefore the effect of the flow perturbation from previous months is considered as negligible. Hence, the number of hydrodynamic transport simulation calls for updating the AL reduced gradient matrix can be reduced

from 576 to 48 for the central-difference method by not simulating the salinity in the bay for the remaining months.

Other test run results indicate that the difference of the computed AL reduced gradients between the forward and the central difference methods is insignificant. The forward difference method is sufficient for the purposes of the AL reduced gradient computations. Thus the number of simulation calls to the hydrodynamic transport model can be further reduced to 24.

The test results indicate that over 95% of the CPU time for the model run is required in the hydrodynamic transport model runs for flow and salinity simulations. Although this dramatical reduction in the number of hydrodynamic transport simulations (from 576 to 24) will save the CPU time significantly, it is still an extremely intensive computational effort for the entire model. The inner optimization model of GRG2 requires 7–60 iterations before the optimal solution is found for the given augmented Lagrangian parameters (initial multiplier, initial penalty, and penalty multiplier). Each iteration may require one or more updates of the reduced gradient and many times for computing the objective functions. The number of the simulation calls is then multiplied by the number of outerloop iterations for updating the augmented Lagrangian parameters and returns to the inner optimizer.

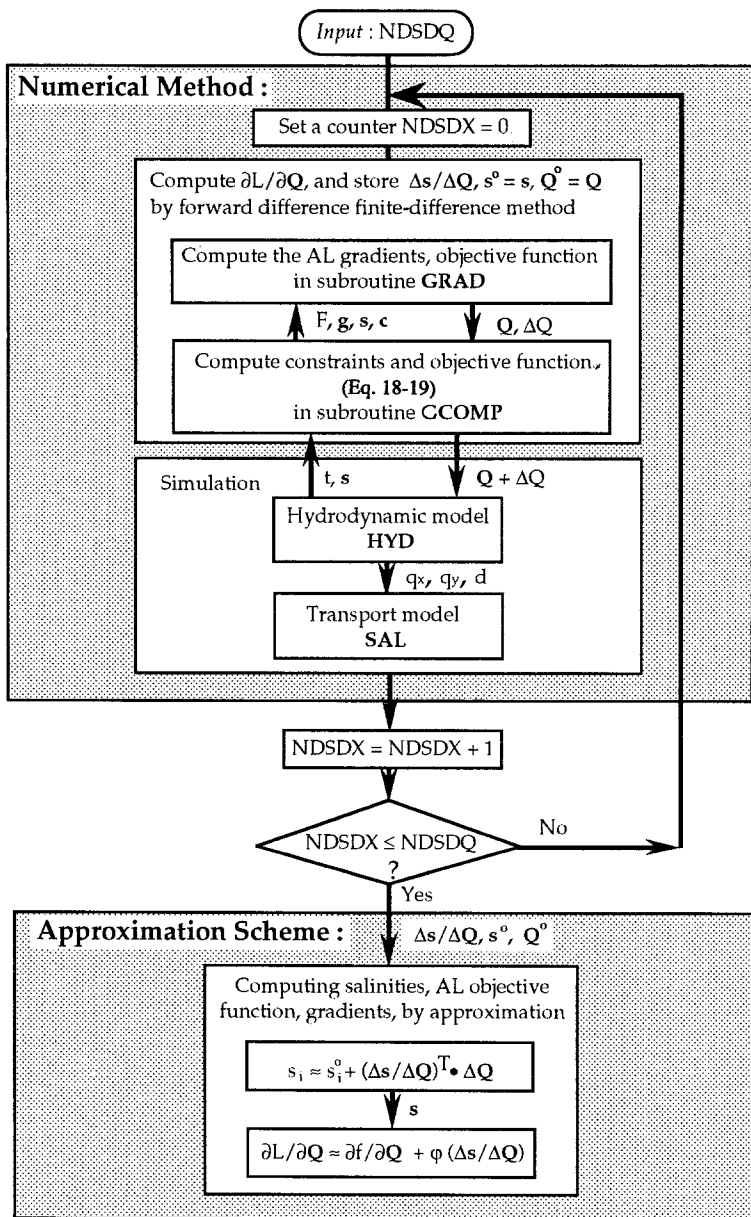
### Gradient Approximation Scheme

The frequent number of simulations requires high CPU times so that innovative modification is needed to reduce the CPU time in simulation. The approximation scheme for computing the AL gradients, presented here, is based on the premise that the change of the salinity derivatives with respect to flow is relatively small compared with the flow changes within a certain flow range. In other words, for a given set of flows, the higher order of salinity derivatives (second partial derivatives) are negligible. This assumption is not proven in theory, but the fact that the linearity in the formed transport PDE (second order, though) and the fully explicit time-centered differencing for the nonlinear hydrodynamic PDE's might suggest that the assumption be a close guess. To verify this assumption, a simulation model was developed to incorporate the hydrodynamic transport model and the finite-difference method for computation of the AL objective gradients. The simulation results show that with change of flow ( $\Delta Q$ ) of 61,675,000 m<sup>3</sup> (50,000 acre-ft), the corresponding change  $\partial s/\partial Q$  usually occurs in the 4th or 5th digits. Although the numerical values obtained from the simulation runs are case-specific, it is reasonable to state that the change of the salinity with respect to flow ( $\partial s/\partial Q$ ) is relatively small compared with the change of inflows.

Fig. 4 is a flowchart of the procedure for the approximation scheme for computing the AL gradients and the objective functions. By the finite-difference method, the gradients of the AL objective function Minimize  $L[s(Q), Q, \sigma, \mu]$  (18), with respect to monthly inflows,  $Q(Q = \{Q_1, Q_2, \dots, Q_n\})$  is computed by the forward-difference method

$$\frac{\partial L}{\partial Q_m} = \frac{L|_{Q_m + \Delta Q_m} - L|_{Q_m}}{\Delta Q_m} \dots \dots \dots (21)$$

for variable element  $Q_m$  ( $m = 1, 2, \dots, n$ ). The simulator is called to compute the AL terms in the objective,  $\sum_i 1_i \{c_i[s_i(Q)], \mu_i, \sigma_i\}$ , (18) by simulating the salinities and computing the salinity violation terms. The re-



**FIG. 4. Flowchart of Approximation Scheme for Computing Gradients and Objective Function**

sultant Jacobian matrix of  $\partial s/\partial Q$  and the vectors of  $s$  and  $Q$  are stored as  $\Delta s/\Delta Q$ ,  $s^0$  and  $Q^0$ .

The approximation scheme can be described as follows. To compute the new AL gradients for flows of  $Q$ , the changes of flow from previous evaluation of  $Q^0$  is simply the difference of the two as

$$\Delta Q = Q^o - Q \dots\dots\dots (22)$$

The associated salinities *s* are computed by

$$s_i = s_i^o + \left( \frac{\Delta s}{\Delta Q} \right)^T \Delta Q \dots\dots\dots (23)$$

and the updated objective function is

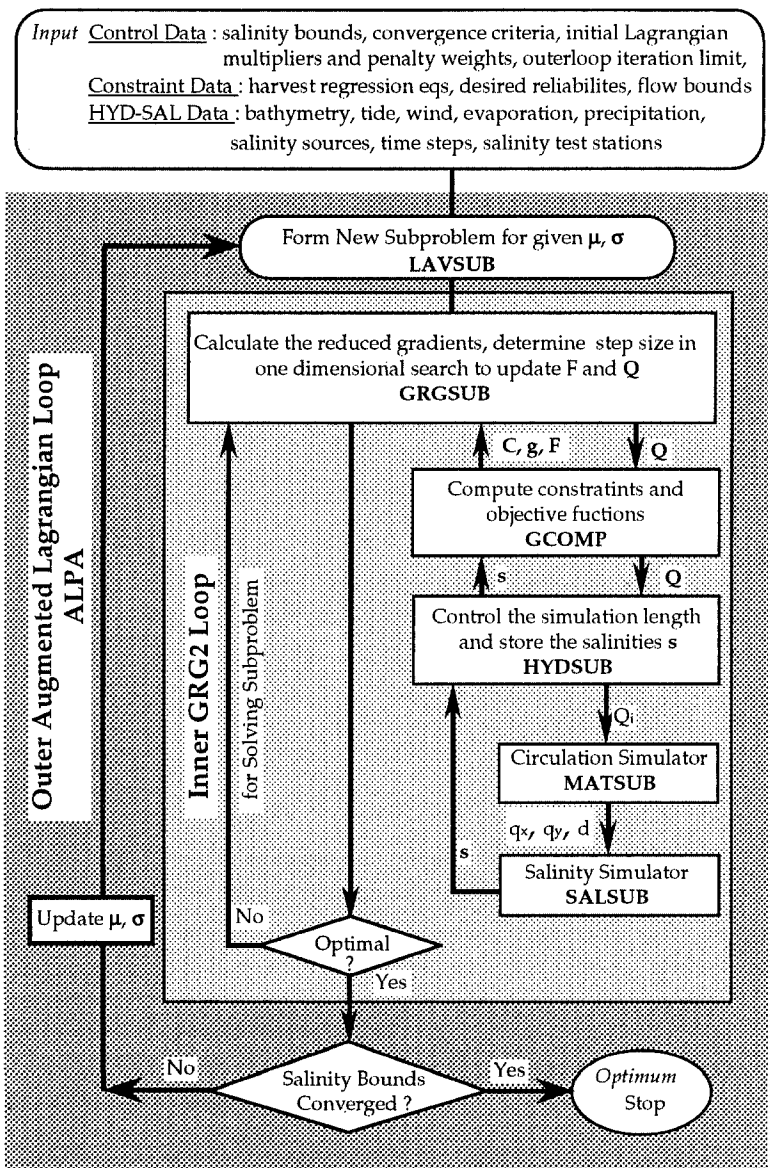


FIG. 5. Flowchart of OPTFLOW

$$L[s(\mathbf{Q}), \mathbf{Q}, \boldsymbol{\mu}, \boldsymbol{\sigma}] = f(\mathbf{Q}) + \sum_i 1_i \{c_i[s_i(\mathbf{Q})], \mu_i, \sigma_i\} \dots\dots\dots (24a)$$

$$L[s(\mathbf{Q}), \mathbf{Q}, \boldsymbol{\mu}, \boldsymbol{\sigma}] = \sum_m Q_m + \sum_i 1_i [c_i(s_i), \mu_i, \sigma_i] \dots\dots\dots (24b)$$

The gradients of the AL objective with respect to the monthly flow are approximated by

$$\frac{\partial L}{\partial \mathbf{Q}} \approx \frac{\partial f}{\partial \mathbf{Q}} + \psi \left( \frac{\Delta \mathbf{s}}{\Delta \mathbf{Q}} \right) \dots\dots\dots (25)$$

where  $\psi$  denotes that the derivative of  $\partial L/\partial \mathbf{Q}$ , (20), is a function of the Jacobian matrix of salinities  $\Delta s/\Delta \mathbf{Q}$ . Once the computation of  $\partial L/\partial \mathbf{Q}$  is completed, the  $\mathbf{s}^o$  and  $\mathbf{Q}^o$  values are updated using  $\mathbf{s}$  and  $\mathbf{Q}$  from the current iteration. A separate computer program was developed to evaluate this approximation scheme for computing the AL objective gradients. The test results indicate that the approximation scheme is extremely efficient with reasonably good accuracy.

**Computer Code**

Bao (1992) developed a computer code, that interfaces GRG2 and HYD-SAL for determining the optimal freshwater inflows to bays and estuaries. A computer model OPTFLOW (optimal flow estuarine model) was developed for application of the general methodology for estuarine water-resources management purposes. OPTFLOW is a modular set of computer programs that consists of five major components: (1) Implementation of the AL algorithm and the approximation scheme for objective reduced gradients; (2) inner optimization module with chance-constrained formulation for fishery harvest constraints; (3) a nonlinear optimizer GRGSUB, which is the standard version of GRG2 with capability of interfacing with other modules; (4) a hydrodynamic module MATSUB, which is a modified version of HYD for simulation of estuarine flows; and (5) a transport module, SALSUB, which is a modified version of SAL for simulating the salinity distribution in the estuary for given flow conditions. The overall structure of OPTFLOW is illustrated in the flowchart (Fig. 5), which consists of several major components.

**SUMMARY**

Estuarine management is defined to maintain the ecologically sound estuarine condition by controlling the amount of freshwater inflow to the estuary. In the past two decades, various hydrodynamic and transport models have been developed and applied to bays and estuaries. Only two previous estuarine management optimization models have been developed (Martin 1987 and Tung et al. 1990). The major drawback in the previous models is using simple regression equations relating freshwater inflow to the salinity as deterministic constraints (Martin 1987) or as chance constraints (Tung et al. 1990).

A general methodology is presented to solve the problems in previous models by replacement of the salinity equations with a two-dimensional hydrodynamic transport model to simulate circulation and temporal and spatial variability of salinity in the bay system. The hydrodynamic transport model HYD-SAL is based on a set of nonlinear partial differential equations for the momentum equations in the *x*- and *y*-directions, continuity equation,

and convective-dispersion of mass balance for transport. Since these equations have to be solved numerically by discretizing in the space and time domains, the resultant optimization problem would be far too large to be solved.

The problem is reduced first by using the simulator to implicitly solve the derived physical equations and further by introducing an augmented Lagrangian method to consider the salinity constraints. The resulting reduced problem is solved by the generalized reduced gradient method. The hydrodynamic transport simulator is modified as submodules to be linked to the nonlinear optimizer to implicitly solve constraint equations for salinity levels.

The solution algorithm for this general methodology can be briefly summarized in two steps. The first step (outerloop iteration) is to determine the augmented Lagrangian (AL) parameters (multiplier and penalty) for each salinity constraint (representing temporal and spatial variability). The second step (inner loop iteration) consists of an optimizer and hydrodynamic transport simulator to solve for the optimum for the given AL parameters. If the salinity convergence criteria are not met, the program goes back to the first step to update the AL parameters, then starts the inner loop iteration again with the updated AL parameters. The two-step (iterations) are repeated until a local optimum is found with all salinity constraints satisfied within the convergence criterion.

A computer model OPTFLOW is developed in the study for application of the general methodology to solve estuarine management problems. In addition to the implementation of the augmented Lagrangian algorithm, the chance-constrained formulation is solved by the OPTFLOW model, which includes an existing hydrodynamic model (HYD), a transport model (SAL), and a nonlinear optimizer (GRG2). OPTFLOW has been applied to the Lavaca-Tres Palacios Estuary in Texas as described in the companion paper, Bao and Mays (1994).

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## APPENDIX I. CHANCE-CONSTRAINT FORMULATION FOR HARVEST EQUATION

The regression equations in the optimization model for harvest are subject to uncertainty due to the variance in the basic data. This uncertainty arises because for the population of observations associated with the sampling process, there is a probability distribution of salinity of commercial harvest for each level of freshwater inflow. The basic application of chance constraints in stochastic programming is to account for the uncertainty of the regression due to random variation in the regression variables by formulating the corresponding constraints into probabilistic form and then transforming them into their deterministic equivalents.

In the problem formulation, these stochastic constraints are transformed into probabilistic statements so that each chance constraint states the prob-

ability that the constraint will be satisfied with a specified reliability level. The harvest constraint (7) can be rewritten in chance-constraint form as

$$P_r(H_k \geq \underline{H}) \geq P_k \quad \dots\dots\dots (26)$$

where the harvest =  $H_k$  is a random variable due to the uncertainty induced by the regression equation (11); and  $P_k$  = desired or required reliability. The chance constraint (26) must be transformed into an equivalent deterministic form in order to implement the optimization algorithm.

The harvest regression equations are either multiple linear models or transformed linear models after logarithmic transformation of  $H_k$  and  $QS_{jm}$  depending upon the species of fish. The commercial fish harvest can be written in a linear or nonlinear form depending upon the species using the regression equations

$$H_k = (\mathbf{QS})_j^T \boldsymbol{\beta}_{H_{kj}} \quad \dots\dots\dots (27)$$

or

$$\ln(H_k) = [\ln(\mathbf{QS})_j]^T \boldsymbol{\beta}_{H_{ki}} \quad \dots\dots\dots (28)$$

The harvest chance constraint (26) is determined using (27) or (28), respectively,

$$P_r[(\mathbf{QS})_j^T \boldsymbol{\beta}_{H_{kj}} \geq \underline{H}_k] \geq P_k \quad \dots\dots\dots (29)$$

or

$$P_r\{[\ln(\mathbf{QS})_j]^T \boldsymbol{\beta}_{H_{ki}} \geq \ln(\underline{H}_k)\} \geq P_k \quad \dots\dots\dots (30)$$

The deterministic form of (29) and (30) are, respectively

$$t_{n-v,1-p_k} \hat{\sigma}_s \sqrt{(\mathbf{QS}_j)^T [(\mathbf{QSD}_j)^T (\mathbf{QSD}_j)^{-1} (\mathbf{QS})_j + 1]} + (\mathbf{QS})_j^T \hat{\boldsymbol{\beta}}_{H_{kj}} \geq H_k \quad \dots\dots\dots (31)$$

and

$$t_{n-v,1-p_k} \hat{\sigma}_{s_{ij}} \sqrt{[\ln(\mathbf{QS})_j]^T \{[\ln(\mathbf{QSD}_j)]^T [\ln(\mathbf{QSD}_j)]\}^{-1} [\ln(\mathbf{QS})_j] + 1} + \ln(\mathbf{QS}_j)^T \hat{\boldsymbol{\beta}}_{H_{ki}} \geq \ln(H_k) \quad \dots\dots\dots (32)$$

where  $t_{n-v,1-p_k}$  = quantile of  $t$  random variable with  $n - v$  degrees of freedom and the probability of  $1 - p_k$ ;  $\hat{\sigma}_{H_k}$  = estimated standard error associated with the harvest regression equations;  $\mathbf{QSD}_j$  = a matrix of the observed data of seasonal freshwater inflow used for the harvest regression equations; and  $\ln(\mathbf{QSD}_j)$  = a matrix in which each element is the logarithmic transform of the corresponding one in  $\mathbf{QSD}_j$ .

The chance-constrained model for various alternatives is obtained by using the associated objective along with constraints (31) and (32), replacing the respective regression relationships.

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### APPENDIX III. NOTATION

*The following symbols are used in this paper:*

- $c_i$  = salinity violation for  $i$ th constraint;  
 $d$  = water depth ( $d = h - z$ );  
 $E_x, E_y$  = horizontal dispersion coefficients in the  $x$ - and  $y$ -directions;  
 $e$  = evaporation rate;  
 $f$  = bottom friction term from Manning equation;  
 $G$  = general salinity constraint;  
 $g$  = gravitational acceleration;  
 $H_k$  = fishery harvest for species  $k$ ;  
 $h$  = water surface elevation;  
 $K$  = wind stress coefficient;  
 $L$  = Lagrangian function;  
 $P_k$  = predetermined probability requirement for  $k$  fish species;  
 $Q$  = freshwater inflow [cfs or acre-ft (1 cfs = 0.0283 m<sup>3</sup>/s; 1 acre-ft = 1,233.5 m<sup>3</sup>)];

- QS** = seasonal flow (independent variable in fishery harvest regression equations);
- QSD<sub>j</sub>** = matrix of the observed data of seasonal freshwater inflow for the fish harvest regression equations;
- q<sub>x</sub>, q<sub>y</sub>** = depth-averaged flow components in the *x*- and *y*-directions per unit width;
- q** = flow per unit width ( $q = \sqrt{q_x^2 + q_y^2}$ );
- r** = rainfall intensity;
- S** = upper bound of salinity;
- S** = lower bound of salinity;
- s** = vertically averaged salinity (ppt);
- t** = time;
- U, V** = net velocities over tidal cycle;
- V<sub>w</sub>** = wind velocity at 10 m above water surface;
- X<sub>w</sub>** = wind stress per unit density of water in *x*-direction ( $X_w = KV_w^2 \cos \theta$ );
- Y<sub>w</sub>** = wind stress per unit density of water in *y*-direction ( $Y_w = KV_w^2 \sin \theta$ );
- x, y** = horizontal Cartesian coordinates;
- z** = bottom elevation;
- β** = coefficient vector for fishery harvest regression equation;
- θ** = wind surface direction with respect to the *x*-axis;
- μ** = Lagrange multiplier vector;
- μ<sub>i</sub>** = Lagrangian multiplier for *i*th salinity constraint;
- σ** = penalty weight vector;
- σ<sub>i</sub>** = penalty weight for *i*th salinity constraint;
- φ** = latitude;
- ω** = angular rotation of the earth; and
- Ω** = Coriolis parameter ( $\Omega = 2\omega \sin \phi$ ).